Evaluation of Gas dynamics of source nozzle geometry by simulation and LDTD-MS/MS experiment

ThP-520

Pierre Picard1, Sarah Demers[1], Jean Lacoursière[1], Jonathan Rochon[1], Mégane Moreau[1], Serge Auger[1]
Phytronix Technologies Inc., Québec, CANADA

Phytronix Breakaway Technologies

OVERVIEW

Purpose

- Design of a new gas focusing system for Laser Diode Thermal Desorption ionization source.

Method

- Numerical simulation of the gas flow of the original LDTD nozzle plate assembly using nonlinear acoustic wave pressure calculation is used to identify possible stagnation points.
- Based on the simulation results, a new geometry is evaluated to reduce the pressure gradient in the key area.
- A modified LDTD nozzle geometry is coupled to a Triple Quadrupole Mass Spectrometer to test different compounds and extractions. The same tests were made using the original geometry for a direct comparison.

Results

- A numerical simulation of the original geometry shows a stagnating pressure close to the inner wall of the edge of the transfer tube.
- New geometry shows a theoretical reduction of 72% in the pressure gradient in the sensitive zone.
- Overall increase in signal of 23% in area counts compared to Luxon model of LDTD-MS/MS

INTRODUCTION

The LDTD ionization source, presented at ASMS 2005, is used in mass spectrometry as an alternative way to introduce samples in a mass spectrometer equipped with an atmospheric inlet. The LDTD uses a nozzle that brings the desorbed molecules to an APCI region for ionization. The nozzle has an optimized gas focusing geometry. The purpose of this work is to review the gas flow properties using nonlinear acoustic wave pressure calculation and evaluate a new geometry. Numerical simulations were correlated by measurements of compounds in LDTD-MS/MS to create an original and updated geometry.

Numerical simulation

Numerical simulation of the gas flow of the original LDTD nozzle plate assembly using nonlinear acoustic waves pressure calculation is used to identify possible stagnation points. Gas flow used of 3 L/min.

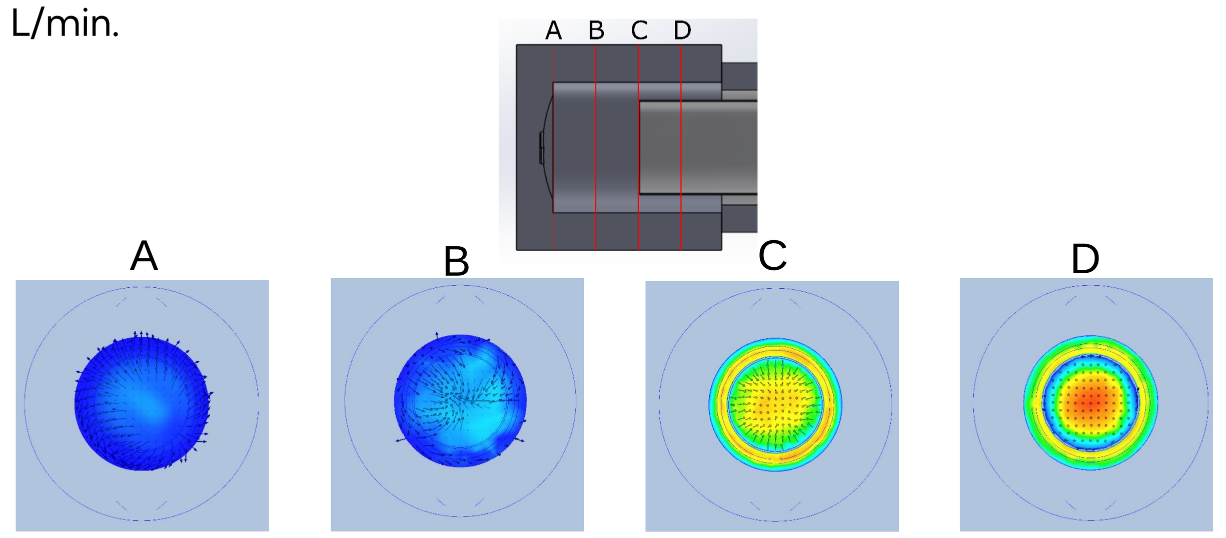

Figure 1

Stagnation point at the surface is represented by scattered flow vector. The flow starts to organize at 2 mm above the surface and is fully developed at 6 mm. Note here that the plume created during the heating cycle is not integrated in the simulation. It improves the flow orientation near the surface.

Using the numerical simulation of the gas flow, a new geometry is conceived to reduce the stagnation points influence and allow the flow to be fully developed near the well surface. The chosen geometry changes the well surface from convex to concave.

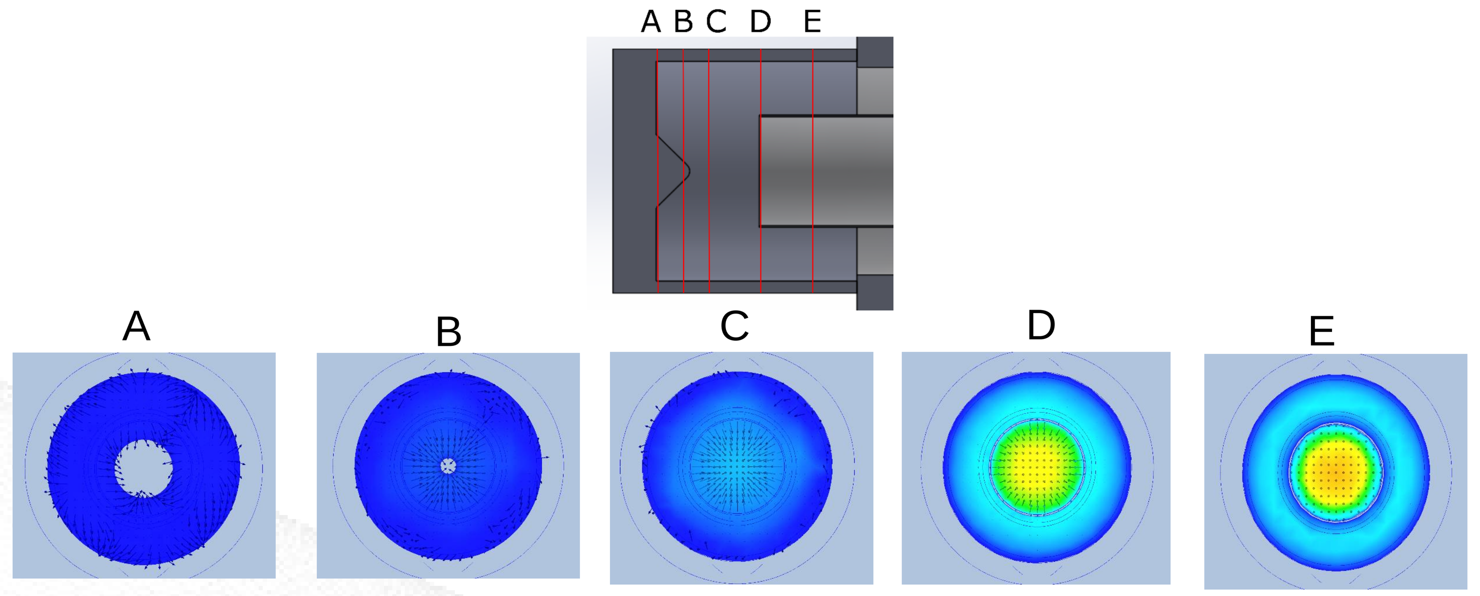

Figure 2

There is no stagnation point visible at the surface. Flow is already organized before reaching the highest point of the surface.

Side view

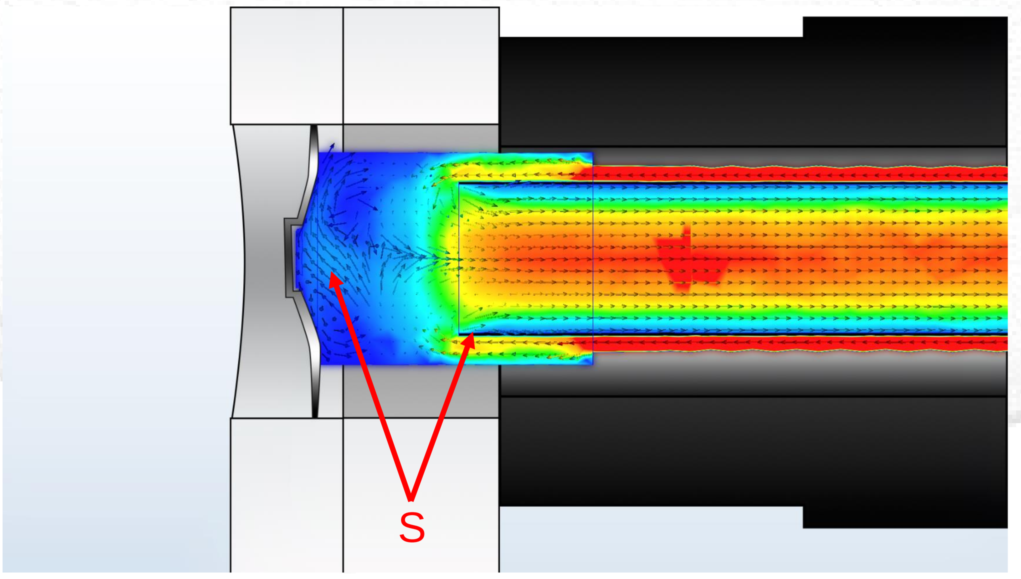

Figure 3

Original LDTD design

- Stagnation zone (S) visible from the surface to 2 mm
- Stagnation point at the border of the transfer tube
- High pressure gradient at transfer tube edge causing turbulent zone

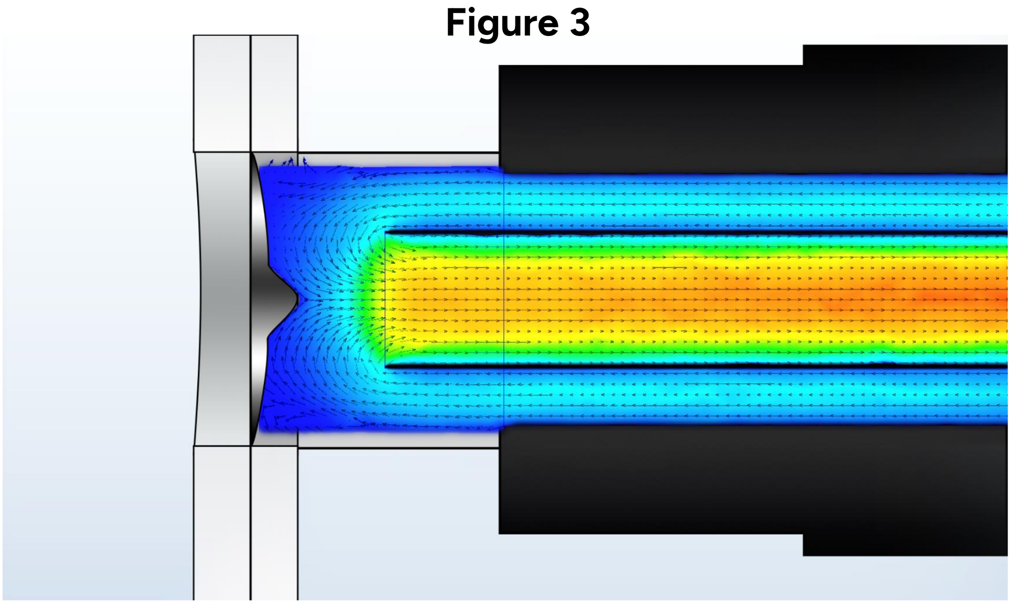

Figure 4

New LDTD design

- Fully developed flow from the surface to 2 mm
- Minimal stagnation point at the border of the transfer tube
- 72% reduction of pressure gradient at transfer tube edge

RESULTS

Measurement of the loss on the first edge of the transfer tube is tested using a Luxon T-960 for the original nozzle and an Axino T-4 for the new design. This instrument includes a system that transforms the convex well shape to a concave shape enabling Uplyft flow design.

- Transfer tubes are thoroughly cleaned prior to a series of 6 consecutive desorptions with a high concentration of Clomiphene LDTD standard at 10 µg/mL. 6 µL are spotted and dried.
- Tubes are disassembled from their instruments.
- Lost compounds on the first 4 mm (figure 5) of the tube is recovered using a methanol water mix (50:50) and quantified by LDTD-MS/MS.
- LDTD original design shows a loss of 2.83%.
- New design with Uplyft flow loss is 1.05% which is a reduction of 63%.

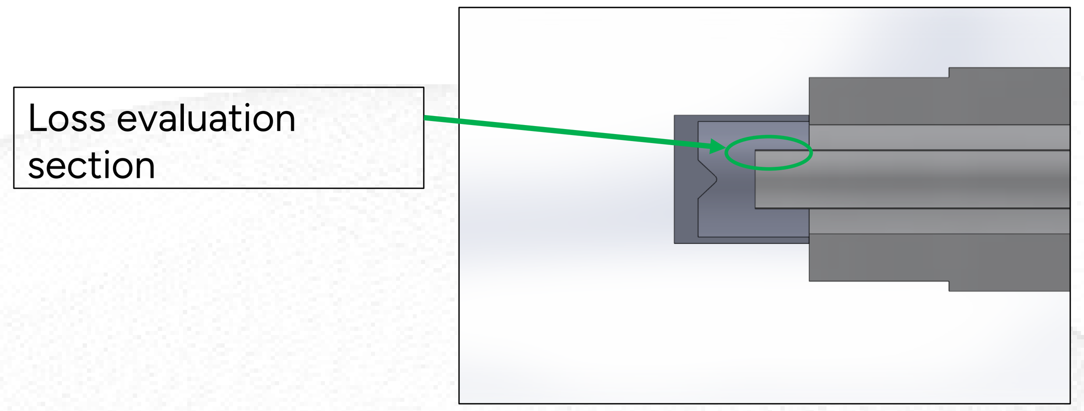

Figure 5

Sensitivity

Sensitivity is established running 12 replicates of LDTD standard using 4 µL of a solution at 1 ng/mL. Both instruments are coupled to the same mass spectrometer, Thermo Vantage, using the same MS method.

- Luxon T-960 (figure 6) for the original nozzle gives 31043 area counts ± 4.0%
- Axino T-4 (figure 7) for the new design gives 40320 area counts ± 5.1%
- Overall sensitivity improvement of 23%.

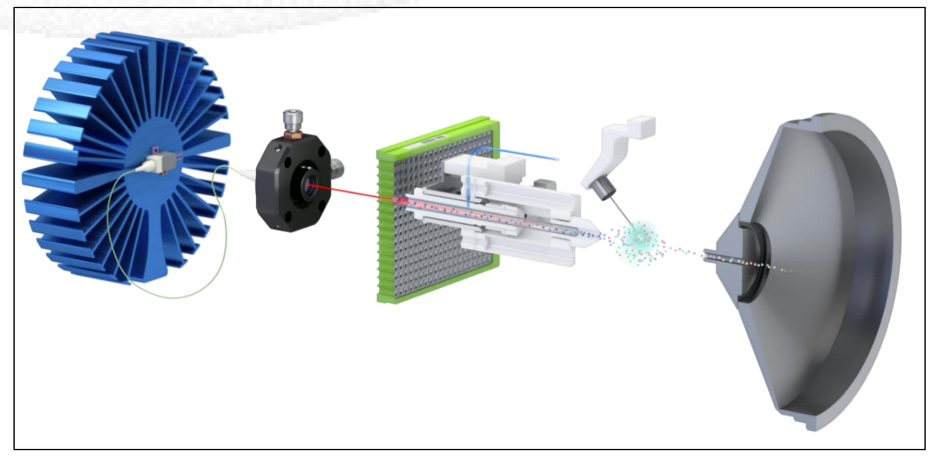

Figure 6

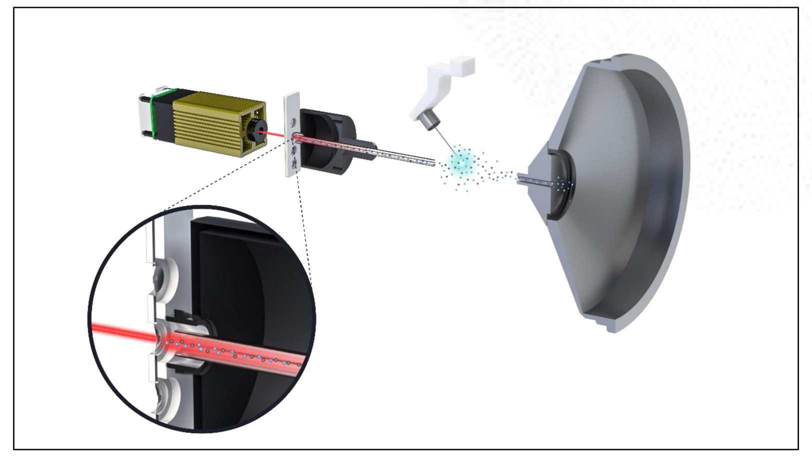

Figure 7

CONCLUSION

- **Numerical simulation of the gas flow of the original LDTD nozzle plate assembly using nonlinear acoustic wave pressure calculation is used to identify stagnation points.**
- **New geometry is evaluated to reduce the pressure gradient in the key area.**
- **New geometry with Uplyft flow shows a theoretical reduction of 72% in the pressure gradient in the sensitive zone.**
- **Overall increase of signal of 23% in area counts compared to Luxon model of LDTD-MS/MS.**